

# Analytical solution of diffusion equation for point defects

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*Abstract.* The analytical solution of the equation describing diffusion of intrinsic point defects has been obtained for a one-dimensional finite-length domain. This solution is intended for investigating and modeling the changes in defect distributions during fabrication of semiconductor devices with layer-type structures. With this purpose, the Robin-type boundary conditions were imposed on both edges of the domain. Using the solution obtained, the calculations of distributions of point defects for different boundary conditions and different defect migration lengths have been carried out. For the case of generation of nonequilibrium point defects due to implantation of hydrogen ions, the influence of the surface on the concentration and spatial distribution of nonequilibrium point defects was investigated depending upon the implantation energy.

*Keywords:* silicon; implantation; annealing; diffusion; modeling

## 1 Introduction

The electrophysical parameters of silicon integrated microcircuits and other semiconductor devices are determined by the state of a defect-impurity system of doped regions. Now, submicron regions of semiconductor devices are formed by means of ions implantation with the subsequent low-budget thermal annealing. During annealing, the main fraction of the nonequilibrium defects generated by ion implantation is eliminated. Because hydrogen atoms readily passivate dangling bonds, introduction of hydrogen into silicon substrates can be used for further improvements in the device performance due to decreasing the imperfections of the crystalline lattice and eliminating undesirable electronic states from the band gap [1]. Introduction of hydrogen can be carried out by means of silicon treatment in a hydrogen containing-plasma [1, 2] or due to implantation of hydrogen ions. In both cases introduction of hydrogen ions is accompanied by generation of additional defects in the near surface region. Due to the smallness of hydrogen atoms, it is found that single point defects, namely, vacancies and self-interstitials, will be generated in undoped silicon. On the other hand, after implantation of a high fluence of hydrogen ions, due to diffusion and quasichemical reactions of generated point defects among themselves, with hydrogen atoms and other imperfections of crystalline lattice, the thin heavily damaged layer, i. e., a quite deep weakened zone, can be formed in the bulk of a semiconductor. As a result, the active layer with SiO<sub>2</sub> isolation can be separated from the rest of the bulk substrate due to splitting which takes place inside the weakened zone. In such a way different structures called silicon-on-insulator (SOI) are formed [3] which have a number of advantages in comparison with the electric isolation fabricated by the traditional technology.

It is worth noting that nonequilibrium point defects can be mobile even at room temperature. Indeed, according to the temperature dependence obtained in the paper

[4], the diffusivity of silicon self-interstitials atoms  $d_i^I = 1.06 \mu\text{m}^2/\text{s}$  for a temperature of 300 K. On the other hand, it follows from the data of [5] that this diffusivity is equal to  $3.2 \times 10^4 \mu\text{m}^2/\text{s}$ . The characteristic diffusion length of silicon self-interstitials  $L^I = \sqrt{d_i^I t}$  obtained for these values of diffusivity varies from  $3.26 \mu\text{m}$  to  $566 \mu\text{m}$  for the time duration  $t = 10 \text{ s}$ . It means that even at room temperature silicon self-interstitials diffuse easily far away from the boundaries of active regions. Thus, distributions of nonequilibrium point defects in fabricated semiconductor devices are determined not only by their generation in the local domains, but also by defect redistribution due to diffusion.

For calculation of distributions of point defects in the paper by Minear et al. [6] the analytical solution of the equation

$$d_i \frac{d^2 C^D}{dx^2} - \frac{C^D}{\tau_i} + G^R(x) = 0 \quad (1)$$

describing diffusion of point defects was obtained on the semiinfinite interval  $[0, +\infty]$ . The case of the constant coefficients  $d_i$  and  $\tau_i$  was considered. Here  $C^D = C^D(x)$  is the concentration of point defects;  $d_i$  and  $\tau_i$  are the diffusivity and the average lifetime of point defects in an intrinsic semiconductor, respectively.

It was supposed in [6] that nonequilibrium point defects were continuously generated during ion implantation of impurity atoms and diffused to the surface and into the bulk of a semiconductor. The surface was considered to be a perfect sink for point defects. The concentration of nonequilibrium defects was also set equal to zero at infinity. It was supposed that the generation of nonequilibrium point defects is determined by two factors, namely, generation due to the primary Rutherford scattering and secondary cascades and generation by hard-sphere interaction at or near the end of ion's track. Then, the total generation rate of point defects in the volume unit can be approximated by an expression with two summands:

$$G^R(x) = G_m^{Ruth} \operatorname{erfc} \left( -\frac{x - R_p}{\Delta R_p} \right) + G_m^R \exp \left[ -\frac{(x - R_p)^2}{2\Delta R_p^2} \right], \quad (2)$$

where  $G_m^{Ruth}$  and  $G_m^R$  are the maximal values of point defect generation rates;  $R_p$  and  $\Delta R_p$  are the average projective range of implanted ions and straggling of the projective range, respectively.

A similar solution was obtained in [7] for the Robin boundary condition on the surface of a semiconductor:

$$-d_i \frac{dC^D}{dx} \Big|_{x=0} + v^S C^D(0) = 0, \quad (3)$$

where  $v^S$  is the parameter describing the velocity of point defect trapping on the surface of a semiconductor. Only the second term in the right-hand side of expression (2) is used for the generation rate of nonequilibrium defects.

At present, in the modern silicon technology, different layered structures such as  $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$  [8, 9, 10] and silicon-on-insulator [3] are widely used. Therefore, it is reasonable to obtain an analytical solution of the equation for diffusion of intrinsic point defects in a finite-length domain  $[0, x_B]$ . The solution obtained can be helpful for studying the

form of point defect distributions under characteristic conditions used in processing semiconductor substrates and for verification of numerical solutions. This solution can be also applied for modeling a number of the processes of diffusion of vacancies and silicon self-interstitial because the parameters describing the transport processes of point defects in silicon and known from the literature differ by many orders of magnitude [11].

## 2 The boundary value-problem for defect diffusion

The diffusion equations for vacancies and silicon self-interstitials that take into account different charge states of intrinsic point defects and drift of the charged species in the built-in electric field were obtained in [12, 13]. These equations have the following form:

### 1) equation of vacancy diffusion

$$\begin{aligned} \nabla \left[ d^V(\chi) \nabla \tilde{C}^{V\times} \right] - \nabla \left[ (\omega^\chi - 1) \frac{\partial d^V(\chi)}{\partial (C - C^B)} \nabla (C - C^B) \tilde{C}^{V\times} \right] + \frac{S^E - G^E}{C_{eq}^{V\times}} \\ - k^{AIkV}(\chi) C^{AIk} \tilde{C}^{V\times} - k^{IV}(\chi) C_{eq}^{I\times} \tilde{C}^{I\times} \tilde{C}^{V\times} - \frac{S^V}{C_{eq}^{V\times}} + \frac{G^{VT} + G^{VR}}{C_{eq}^{V\times}} = 0 \end{aligned} \quad , \quad (4)$$

### 2) equation for diffusion of silicon self-interstitial

$$\begin{aligned} \nabla \left[ d^I(\chi) \nabla \tilde{C}^{I\times} \right] - \nabla \left[ (\omega^\chi - 1) \frac{\partial d^I(\chi)}{\partial (C - C^B)} \nabla (C - C^B) \tilde{C}^{I\times} \right] + \frac{S^F - G^F}{C_{eq}^{I\times}} \\ - k^W(\chi) \tilde{C}^{I\times} + \frac{k^{AIk}}{C_{eq}^{I\times}} C^{AIk} - k^{IV}(\chi) C_{eq}^{V\times} \tilde{C}^{V\times} \tilde{C}^{I\times} - \frac{S^I}{C_{eq}^{I\times}} + \frac{G^{IT} + G^{IR}}{C_{eq}^{I\times}} = 0 \end{aligned} \quad , \quad (5)$$

where

$$\omega^\chi = \frac{\chi}{k_B T} \frac{\partial \mu^\chi}{\partial \chi} . \quad (6)$$

Here  $\tilde{C}^{V\times}$  and  $\tilde{C}^{I\times}$  are respectively the concentrations of nonequilibrium vacancies and silicon self-interstitials in the neutral charge state, normalized to the equilibrium concentrations of these species  $\tilde{C}_{eq}^{V\times}$  and  $\tilde{C}_{eq}^{I\times}$ ;  $C$  and  $C^B$  are the concentrations of substitutionally dissolved impurity and impurity with the opposite-type of conductivity, respectively;  $C^{AIk}$  is the concentration of impurity interstitials with the charge state  $k$ ;  $\chi$  is the concentration of charge carriers (electrons  $n$  or holes  $p$  for doping with donor or acceptor impurities, respectively) normalized to the intrinsic concentration of charge carriers  $n_i$ ;  $\omega^\chi$  is the function which describes a deviation of an electron (hole) system beyond the perfect solubility;  $\mu^\chi$  is the chemical potential of electrons (holes);  $d^V(\chi)$  is the effective diffusivity of vacancies;  $k^{AIkV}$  and  $k^{IV}$  are respectively the effective recombination coefficients of impurity interstitials (in a charge state  $k$ ) and silicon self-interstitials with vacancies;  $G^E$  and  $S^E$  are the rates of generation and dissolution of the “impurity atom – vacancy” pairs;  $S^V$  is the rate of the trapping of the vacancies on the immobile

imperfections of a crystalline lattice;  $G^{VT}$  and  $G^{VR}$  are the rates of thermal generation of vacancies and generation of the vacancies due to external irradiation;  $d^I(\chi)$  is the effective diffusivity of silicon self-interstitials;  $k^W$  is the effective coefficient of the replacement of the impurity atom by self-interstitial from the substitutional position into the interstitial one (Watkins effect [14]);  $k^{AIk}$  is the effective coefficient for conversion of impurity atoms from an interstitial to the substitutional position (phenomenon opposite to the Watkins effect);  $G^F$  and  $S^F$  are the rates of generation and dissolution of the “impurity atom – silicon self-interstitial” pairs;  $S^I$  is the rate of the trapping of the silicon self-interstitials on the immobile sinks of a crystalline lattice;  $G^{IT}$  and  $G^{IR}$  are the rates of a thermal generation of silicon self-interstitials and their generation due to external irradiation.

The diffusion equations obtained have the following characteristic features:

(i) these two equations describe diffusion of all point defects with different charge states as a whole, although only the concentration of the neutral vacancies  $\tilde{C}^{V\times}$  and silicon self-interstitials  $\tilde{C}^{I\times}$  must be derived to solve equations (4) and (5), respectively. After the solution, the distributions of charged species, namely, vacancies in a charge state  $r$  and silicon self-interstitials in a charge state  $q$ , can be calculated from the expressions describing the local thermodynamic equilibrium  $C^{Vr} = \tilde{C}^{V\times} C_{eq}^{V\times} h^{Vr} \chi^{-zz^{Vr}}$  and  $C^{Iq} = \tilde{C}^{I\times} C_{eq}^{I\times} h^{Iq} \chi^{-zz^{Iq}}$ . Here  $z$ ,  $z^{Vr}$ , and  $z^{Ir}$  are respectively the charge of a substitutional impurity atom, the charge of a vacancy in the charge state  $r$ , and the charge of a silicon self-interstitial in the charge state  $q$  in terms of the elementary charge;  $h^{Vr}$  and  $h^{Iq}$  are the constants of the mass action law for reactions of defects conversion from neutral to nonzero charge states;

(ii) the equations obtained take into account the drift of all charged species due to the built-in electric field. At the same time, there is no explicit term that would describe the drift and be proportional to the first derivative of the concentration of mobile species that essentially complicates the numerical solution. To exclude this term, a system of equations describing diffusion of intrinsic point defects in each charge state was written. Then, the special mathematical transformations of these equations were performed using the mass action law for conversions between different charge states of vacancies and self-interstitials. As a result of these transformations, the drift of vacancies and silicon self-interstitials in the electric field are taken into account in the effective diffusion coefficients  $d^V(\chi)$  and  $d^I(\chi)$ ;

(iii) the effective diffusion coefficients  $d^V(\chi)$  and  $d^I(\chi)$  as well as the effective coefficients of quasichemical reactions  $k^W(\chi)$ ,  $k^{AIkV}(\chi)$ , and  $k^{IV}(\chi)$  are smooth and monotone functions of the concentration of dopant atoms.

It is to be noted that equations (4) and (5) are very convenient for numerical solution and studying the fundamentals of diffusion processes owing to the features (i), (ii), and (iii). In addition, it follows from these equations that for defect diffusion in intrinsic or homogeneously doped semiconductor all nonlinear coefficients are converted into constants. Then, equations (4) and (5) can be presented for a one-dimensional (1D) domain in the form

$$d_i \frac{d^2 \tilde{C}^\times}{dx^2} - \frac{\tilde{C}^\times}{\tau} + \frac{G^T + G^R}{C_{eq}^\times} = 0 \quad , \quad (7)$$

where  $d_i$  and  $\tau$  are the diffusivity and the average lifetime of point defects in intrinsic

silicon (we do not concretize the defect species).

In a number of cases concerning the impurity and point defect diffusion, it is possible to neglect the mutual interactions of vacancies and interstitial atoms. For example, under a low-temperature oxidation of the surface of a semiconductor, silicon self-interstitials are the dominating defects in a silicon crystal [15]. Therefore, one can neglect calculation of vacancy distribution in modeling the processes of impurity diffusion due to negligible vacancy concentration. In this case, the average lifetime of other defects (silicon self-interstitials) can be assumed to be constant  $\tau = \tau_i = \text{const}$ . Here  $\tau_i$  is the average lifetime of defects in an intrinsic semiconductor under equilibrium conditions. Using the quantity of the average migration length of point defects  $l_i = \sqrt{d_i \tau_i}$ , one can present the equation of diffusion (7) in the following form:

$$\frac{d^2 \tilde{C}^\times}{dx^2} - \frac{1}{l_i^2} \tilde{C}^\times + \frac{1 + \tilde{g}(x, t)}{l_i^2} = 0 \quad , \quad (8)$$

where  $\tilde{g}(x, t) = G^R/G^T$  represents the generation rate of point defects under consideration in the volume unit of a semiconductor normalized to the thermal generation rate of these defects.

Let us obtain a solution of equation (8) in the 1D finite-length domain  $[0, x_B]$  for  $\tilde{g}(x, t) = \tilde{g}(x)$  and the Robin boundary conditions on the left and right boundaries:

$$-w_1^S d_i \frac{d\tilde{C}^\times}{dx} \Big|_{x=0} + w_2^S \tilde{C}^\times(0) = w_3^S \quad , \quad (9)$$

$$-w_1^B d_i \frac{d\tilde{C}^\times}{dx} \Big|_{x=x_B} + w_2^B \tilde{C}^\times(x_B) = w_3^B \quad , \quad (10)$$

where  $w_1^S$ ,  $w_2^S$ ,  $w_3^S$ ,  $w_1^B$ ,  $w_2^B$ , and  $w_3^B$  are the constant coefficients specifying the concrete type of real boundary conditions.

### 3 Solution of the equation describing defect diffusion

For the solution of the boundary-value problem (8), (9), and (10) we can use the Green function approach [16]:

$$\tilde{C}^\times(x, t) = \int_0^{x_B} G(x, \xi) \omega(\xi) d\xi \quad , \quad (11)$$

where the standardizing function  $\omega(\xi)$  has the following form:

$$\omega(\xi) = \frac{1 + \tilde{g}(x, t)}{l_i^2} + \omega_S(\xi) + \omega_B(\xi) \quad (12)$$

and  $G(x, \xi)$  is the Green's function for equation (8). Using the standardizing function  $\omega(\xi)$  [16] allows one to reduce the previous boundary-value problem to the boundary-value problem with boundary conditions having zero right hand sides:

$$- w_1^S d_i \frac{d \tilde{C}^\times}{dx} \Big|_{x=0} + w_2^S \tilde{C}^\times(0) = 0 \quad , \quad (13)$$

$$- w_1^B d_i \frac{d \tilde{C}^\times}{dx} \Big|_{x=x_B} + w_2^B \tilde{C}^\times(x_B) = 0 \quad . \quad (14)$$

The Green function for equation (15) with boundary conditions (13) and (14) has the following form [16]:

$$G(x, \xi) = \frac{1}{K} \begin{cases} Q_1(x) Q_2(\xi) & 0 \leq x \leq \xi \leq x_B \\ Q_1(\xi) Q_2(x) & 0 \leq \xi \leq x \leq x_B \end{cases} \quad , \quad (15)$$

where

$$K = -[Q_1(x)Q_2'(x) - Q_2(x)Q_1'(x)] = \text{const} \quad . \quad (16)$$

Here  $Q_1(x)$  and  $Q_2(x)$  are the linearly independent solutions of the homogeneous equation

$$\frac{d^2 \tilde{C}^\times}{dx^2} - \frac{1}{l_i^2} \tilde{C}^\times = 0 \quad . \quad (17)$$

with the following conditions on the left boundary:

$$Q_1(0) = -w_1^S d_i \quad , \quad Q_1'(0) = -w_2^S \quad (18)$$

and on the right one:

$$Q_2(x_B) = -w_1^B d_i \quad , \quad Q_2'(x_B) = -w_2^B . \quad (19)$$

Taking into account [16], we can write the functions  $\omega_S(x)$  and  $\omega_B(x)$  as

$$\omega_S(x) = \begin{cases} \frac{1}{w_1^S d_i} \delta(-x) w_3^S, & w_1^S \neq 0 \\ \frac{1}{w_2^S} \delta'(-x) w_3^S, & w_2^S \neq 0 \end{cases} \quad , \quad (20)$$

$$\omega_B(x) = \begin{cases} -\frac{1}{w_1^B d_i} \delta(x_B - x) w_3^B, & w_1^B \neq 0 \\ -\frac{1}{w_2^B} \delta'(x_B - x) w_3^B, & w_2^B \neq 0 \end{cases} . \quad (21)$$

Let us consider the following Robin boundary condition on the left boundary of the layer (for example, on the surface  $x = 0$ ) and in the bulk of a semiconductor  $x = x_B$ :

$$w_1^S = 1 \quad , \quad w_2^S \neq 0 \quad , \quad w_3^S = 0 \quad , \quad (22)$$

$$w_1^B = 1 \quad , \quad w_2^B \neq 0 \quad , \quad w_3^B = 0 \quad . \quad (23)$$

These boundary conditions are very interesting for technology because they allow one to describe the flux of point defects through the left and the right boundaries as well as

the absorption of defects on the boundary [7]. It follows from (22) and (23) that  $\omega_S(x) = 0$  and  $\omega_B(x) = 0$ , whereas the solutions  $Q_1$  and  $Q_2$  have the following form:

$$Q_1(x) = -\frac{1}{2} \left[ (d_i + l_i w_2^S) e^{\frac{x}{l_i}} + (d_i - l_i w_2^S) e^{-\frac{x}{l_i}} \right] , \quad (24)$$

$$Q_2(x) = -\frac{1}{2} \left[ (d_i - l_i w_2^B) e^{\frac{x_B - x}{l_i}} + (d_i + l_i w_2^B) e^{-\frac{x_B - x}{l_i}} \right] . \quad (25)$$

Then, the constant  $K$  is equal to

$$K = -\frac{1}{2l_i} \left[ (d_i - l_i w_2^B) (d_i + l_i w_2^S) e^{\frac{x_B}{l_i}} - (d_i + l_i w_2^B) (d_i - l_i w_2^S) e^{-\frac{x_B}{l_i}} \right] . \quad (26)$$

and the Green function has the following form:

$$G(x, \xi) = -\frac{l_i}{2 \left[ (d_i - l_i w_2^B) (d_i + l_i w_2^S) e^{\frac{x_B}{l_i}} - (d_i + l_i w_2^B) (d_i - l_i w_2^S) e^{-\frac{x_B}{l_i}} \right]} \times \begin{cases} \left[ (d_i + l_i w_2^S) e^{\frac{x}{l_i}} + (d_i - l_i w_2^S) e^{-\frac{x}{l_i}} \right] \\ \times \left[ (d_i - l_i w_2^B) e^{\frac{x_B - \xi}{l_i}} + (d_i + l_i w_2^B) e^{-\frac{x_B - \xi}{l_i}} \right] & 0 \leq x \leq \xi \leq x_B , \\ \left[ (d_i + l_i w_2^S) e^{\frac{\xi}{l_i}} + (d_i - l_i w_2^S) e^{-\frac{\xi}{l_i}} \right] \\ \times \left[ (d_i - l_i w_2^B) e^{\frac{x_B - x}{l_i}} + (d_i + l_i w_2^B) e^{-\frac{x_B - x}{l_i}} \right] & 0 \leq \xi \leq x \leq x_B . \end{cases} \quad (27)$$

Let us assume that a generation of nonequilibrium point defects occurs due to ion implantation and that the distribution of their generation rate is approximated by the Gaussian function:

$$\tilde{g}(x, t) = g_m \exp \left[ -\frac{(x - R_{pd})^2}{2\Delta R_{pd}^2} \right] , \quad (28)$$

where  $g_m$  is the maximum rate of generation of nonequilibrium defects normalized to the rate of the thermal generation of this species;  $R_{pd}$  is the position of the generation maximum and  $\Delta R_{pd}$  is the standard deviation.

Substituting the Green function (27) and expression (28) into (11) allows one to obtain a spatial distribution of point defect concentration:

$$\tilde{C}^\times(x) = \tilde{C}_{eq}^\times(x) + \tilde{C}_R^\times(x) , \quad (29)$$

where  $\tilde{C}_{eq}^\times(x)$  is the distribution of point defect concentration in the case of zero external radiation and  $\tilde{C}_R^\times(x)$  is the change of defect concentration due to ion implantation:

$$\begin{aligned}
\tilde{C}_{eq}^\times(x) = & \left\{ (d_i - l_i w_2^S) (d_i + l_i w_2^B) - (d_i + l_i w_2^S) (d_i - l_i w_2^B) e^{\frac{2x_B}{l_i}} \right. \\
& + \left[ (d_i + l_i w_2^B) l_i w_2^S - (d_i + l_i w_2^S) l_i w_2^B e^{\frac{x_B}{l_i}} \right] e^{\frac{x}{l_i}} \\
& + \left[ (d_i - l_i w_2^B) l_i w_2^S e^{\frac{2x_B}{l_i}} - (d_i - l_i w_2^S) l_i w_2^B e^{\frac{x_B}{l_i}} \right] e^{-\frac{x}{l_i}} \Bigg\} \\
& \times [(d_i - l_i w_2^S) (d_i + l_i w_2^B) - (d_i + l_i w_2^S) (d_i - l_i w_2^B)]^{-1}
\end{aligned} \tag{30}$$

and

$$\tilde{C}_R^\times(x) = \tilde{C}_{R1}^\times(x) + \tilde{C}_{R2}^\times(x) \quad , \tag{31}$$

where

$$\begin{aligned}
\tilde{C}_{R1}^\times(x) = & g_m \sqrt{\frac{\pi}{2}} \frac{\Delta R_{pd}}{2l_i} e^{\frac{\Delta R_{pd}^2 - 2l_i R_{pd} + 2l_i x_B}{2l_i^2}} \\
& \times \left[ (d_i - l_i w_2^B) e^{\frac{x_B - x}{l_i}} + (d_i + l_i w_2^B) e^{-\frac{x_B - x}{l_i}} \right] \\
& \times \left\{ (d_i + l_i w_2^S) e^{\frac{2R_{pd}}{l_i}} \left[ erf \left( \frac{\Delta R_{pd}^2 + l_i R_{pd} - l_i x}{\sqrt{2} \Delta R_{pd} l_i} \right) - erf \left( \frac{\Delta R_{pd}^2 + l_i R_{pd}}{\sqrt{2} \Delta R_{pd} l_i} \right) \right] \right. \\
& + (d_i - l_i w_2^S) \left[ erf \left( \frac{\Delta R_{pd}^2 - l_i R_{pd}}{\sqrt{2} \Delta R_{pd} l_i} \right) - erf \left( \frac{\Delta R_{pd}^2 - l_i R_{pd} + l_i x}{\sqrt{2} \Delta R_{pd} l_i} \right) \right] \Bigg\} \\
& \times \left[ (d_i - l_i w_2^S) (d_i + l_i w_2^B) - (d_i + l_i w_2^S) (d_i - l_i w_2^B) e^{\frac{2x_B}{l_i}} \right]^{-1} ,
\end{aligned} \tag{32}$$



$$\begin{aligned}
\tilde{C}_{R2}^{\times}(x) = & g_m \sqrt{\frac{\pi}{2}} \frac{\Delta R_{pd}}{2l_i} e^{\frac{\Delta R_{pd}^2 - 2l_i R_{pd} - 2l_i x}{2l_i^2}} \left[ d_i - l_i w_2^S + (d_i + l_i w_2^S) e^{\frac{2x}{l_i}} \right] \\
& \times \left\{ (d_i + l_i w_2^B) e^{\frac{2R_{pd}}{l_i}} \left[ \operatorname{erf} \left( \frac{\Delta R_{pd}^2 + l_i R_{pd} - l_i x_B}{\sqrt{2} \Delta R_{pd} l_i} \right) - \operatorname{erf} \left( \frac{\Delta R_{pd}^2 + l_i R_{pd} - l_i x}{\sqrt{2} \Delta R_{pd} l_i} \right) \right] \right. \\
& + (d_i - l_i w_2^B) e^{\frac{2x_B}{l_i}} \left[ \operatorname{erf} \left( \frac{\Delta R_{pd}^2 - l_i R_{pd} + l_i x}{\sqrt{2} \Delta R_{pd} l_i} \right) - \operatorname{erf} \left( \frac{\Delta R_{pd}^2 - l_i R_{pd} + l_i x_B}{\sqrt{2} \Delta R_{pd} l_i} \right) \right] \left. \right\} \\
& \times \left[ (d_i - l_i w_2^S) (d_i + l_i w_2^B) - (d_i + l_i w_2^S) (d_i - l_i w_2^B) e^{\frac{2x_B}{l_i}} \right]^{-1}.
\end{aligned} \tag{33}$$

It was mentioned above that in the up-to-date electronics different layered structures such as  $\text{Ge}_x\text{Si}_{1-x}/\text{Si}$  or silicon-on-insulator (SOI) are often used for decreasing the device dimensions and improving the device performance. The derived analytical solution for a finite-length domain  $[0, x_B]$  is convenient for modeling and investigating point defect diffusion in a separate layer of these structures. For example, in Fig. 1 the calculated distribution of point defects in the silicon layer of thickness  $0.4 \mu\text{m}$  is presented. Primarily, the case of zero external radiation ( $g_m = 0$ ) is considered for the better understanding of the influence of ion implantation.

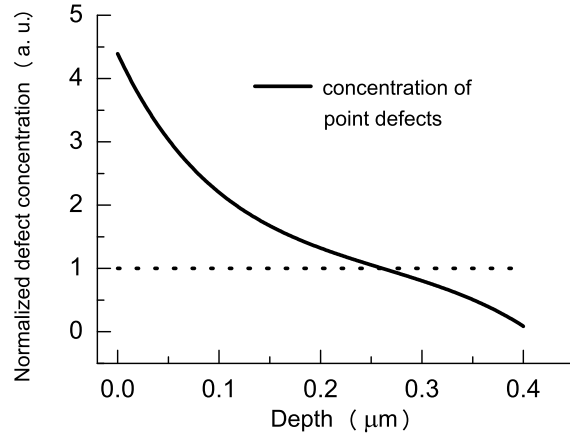


Figure 1: Calculated concentration distribution of the neutral point defects in a silicon layer of thickness  $0.4 \mu\text{m}$ . The dotted curve represents the thermally equilibrium value of the normalized concentration of neutral point defects

It is evident that for zero fluxes of defects through the boundaries of the layer a distribution of point defects is homogeneous and the value of normalized concentration of these defects is equal to 1 (dotted curve). Deviation from the uniform defect distribution

occurs only if there are nonzero fluxes of defects through the boundaries or there is an absorption (generation) of point defects on the surface or at the interface. For example, the distribution of defects presented in Fig. 1 is calculated under the assumption that two fluxes of point defects through the left and right boundaries are directed along the  $x$  axis. With this purpose the coefficients  $w_2^S$  and  $w_2^B$  have been presented in the following form:

$$w_2^S = v_{eff}^S, \quad w_2^B = -v_{eff}^B, \quad (34)$$

where  $v_{eff}^S$  and  $v_{eff}^B$  are the effective rate of point defect removal outside the layer through the left and right boundaries, respectively. For defect distribution presented in Fig. 1, the values  $v_{eff}^S = -0.0094 \mu\text{m/s}$  and  $v_{eff}^B = 4.0 \mu\text{m/s}$  were used. Also, the value of the average migration length of point defects  $l_i = 0.1 \mu\text{m}$  and the value of intrinsic diffusivity  $d_i = 0.01 \mu\text{m}^2/\text{s}$  were chosen. It can be seen from Fig. 1 that according to the boundary conditions (34) used for solving equation (8) the concentration of the point defects in the vicinity of the left boundary increases due to supplying additional defects in the layer, whereas near to the right boundary the concentration of intrinsic point defects decreases due to the removal of this species outside the layer. The analytical solution obtained describes the distribution of the concentration of point defects in the neutral charge state. The concentration of the charged defect species  $C^r(x)$  can be calculated from the above-mentioned expressions  $C^{Vr} = \tilde{C}^{V \times} C_{eq}^{V \times} h^{Vr} \chi^{-zz^{Vr}}$  and  $C^{Iq} = \tilde{C}^{I \times} C_{eq}^{I \times} h^{Iq} \chi^{-zz^{Iq}}$  that follow from the mass action law.

It is worth noting that due to the quasi-stationarity of the diffusion equation for point defects, exactly the same solution takes place for the Dirichlet boundary conditions with  $\tilde{C}^\times(0) = \tilde{C}_S^\times = 4.393$  a.u. and  $\tilde{C}^\times(x_B) = \tilde{C}_B^\times = 0.08689$  a.u. Here  $\tilde{C}_S^\times$  and  $\tilde{C}_B^\times$  are the normalized concentrations of intrinsic point defects on the left (surface) and right boundaries of the layer.

Let us consider now the main features of the solutions of equation (8) in the case of intense generation of nonequilibrium point defects in the vicinity of the surface. Such generation can occur during low-energy implantation of hydrogen ions into semiconductor substrate. For example, let us suppose that the energy of hydrogen implantation is 2 keV. Then, calculation performed by the code SRIM [17] gives the following values:  $R_{pd} = 0.033 \mu\text{m}$ ,  $\Delta R_{pd} = 0.0248 \mu\text{m}$ , if one assumes that the distribution of generated defects is proportional to the distribution of implanted hydrogen ions.

In Fig. 2 the calculated concentration distribution of nonequilibrium point defects in the silicon layer of thickness  $0.4 \mu\text{m}$  is presented. It was supposed that the maximal generation rate of point defects due to the ion implantation exceeds 1000 times the rate of thermal generation ( $g_m = 1000$ ), whereas the diffusion parameters are the same ( $l_i = 0.1 \mu\text{m}$ ,  $d_i = 0.01 \mu\text{m}^2/\text{s}$ ). For comparison, the point defect distribution calculated for the value  $l_i = 0.2 \mu\text{m}$  is also presented. The case of zero fluxes through the left and right boundaries is investigated primarily.

It follows from Fig. 2 that the point defect concentration decreases 1.6 times at the surface of a semiconductor if the average migration length increases 2 times. Simultaneously, the distribution of point defects becomes flatter. On the other hand, there is a significant increase of the point defect concentration, more accurately by a factor of 3.4, on the right boundary of the layer.

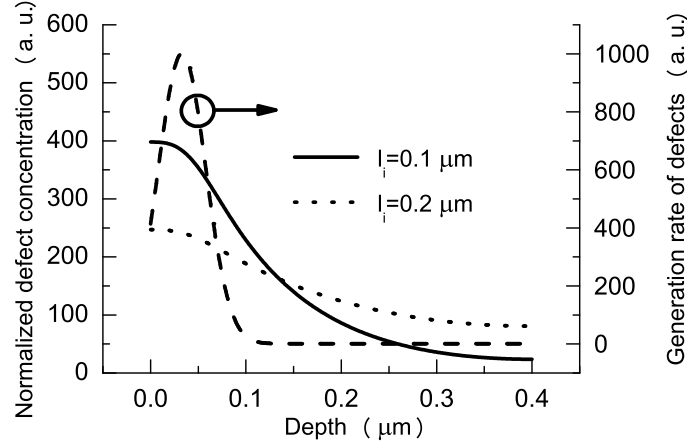


Figure 2: Concentration distribution of the neutral point defects normalized to the thermally equilibrium value of defect concentration in a silicon layer of thickness  $0.4 \mu\text{m}$  for the case of hydrogen implantation with an energy of 2 keV. The dashed line represents the generation rate of point defects normalized to the equilibrium one

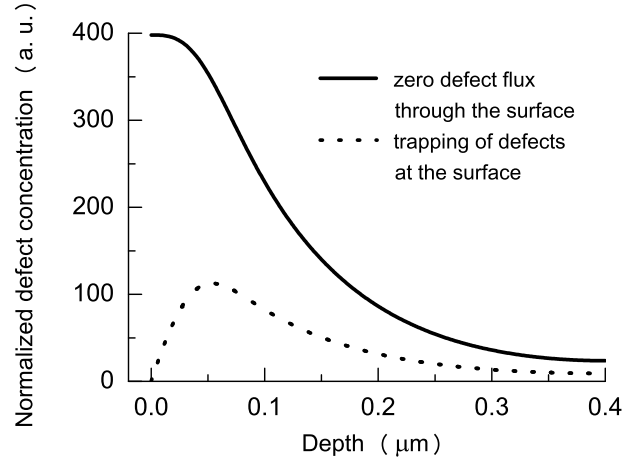


Figure 3: Concentration distribution of the neutral point defects normalized to the thermally equilibrium value of defect concentration in a silicon layer of thickness  $0.4 \mu\text{m}$  for the case of hydrogen implantation with an energy of 2 keV. The solid line represents distribution of point defects calculated for the case of zero defect flux through the left boundary, whereas the dotted line describes diffusion of point defects under conditions of defect trapping on the surface

Now, this paper investigates the main features of the solution obtained for the case of defect removal through the left boundary of the layer. It was mentioned above that this boundary condition is also similar to defect trapping on the surface of a semiconductor. With this purpose Fig. 3 presents two distributions of defects which were calculated for the case of zero defect flux through the left boundary and for the case of intensive trapping

of defects by the surface, respectively. It is supposed that the average migration length of point defects is equal to  $0.1 \mu\text{m}$ . It can be seen from Fig. 3 that the trapping of point defects on the surface results in the change of the form of its concentration profile and in the significant decrease of defect concentration. For example, the maximal concentration of point defects decreases 3.5 times.

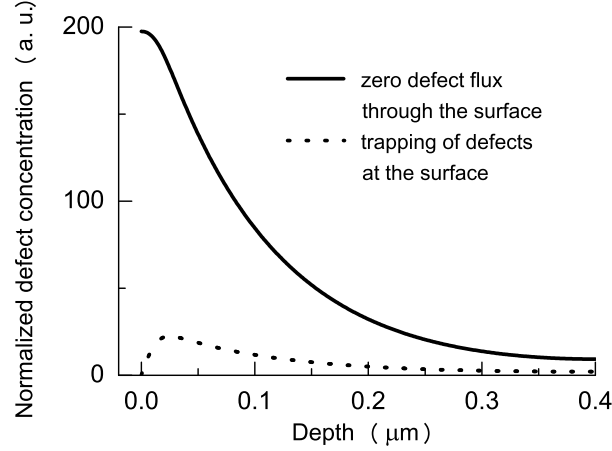


Figure 4: Concentration distribution of the neutral point defects normalized to the thermally equilibrium value of defect concentration in a silicon layer of thickness  $0.4 \mu\text{m}$  for the case of hydrogen implantation with an energy of 500 eV. The solid line represents distribution of point defects calculated for the case of zero defect flux through the left boundary, whereas the dotted line describes diffusion of point defects under conditions of defect trapping on the surface

More serious influence of the surface on the distribution of point defects can be observed for small values of implantation energy. It can be seen from Fig. 4, where a similar calculation for the energy of implantation of hydrogen ions equals to 500 eV is presented. For this value of hydrogen implantation energy the calculation of the parameters describing the distribution of implanted ions gives the following values:  $R_{pd} = 0.0097 \mu\text{m}$ ,  $\Delta R_{pd} = 0.011 \mu\text{m}$  [17].

It can be seen from Fig. 4 that the maximal concentration of point defects decreases 8.8 times due to the trapping of point defects on the surface, which is in close vicinity (a few nanometers) to the region of intense generation of nonequilibrium point defects.

## 4 Conclusions

The analytical solution of the one-dimensional equation that describes quasi-stationary diffusion of intrinsic point defects in semiconductor crystals has been obtained for the case of the Robin boundary conditions on the left and right boundaries of the layer. It is supposed that the generation rate of nonequilibrium point defects is approximated by the Gaussian function. To derive an analytical solution of this boundary-value problem, the Green function approach has been used.

The solution obtained is focused on the application in modeling technological processes used for fabrication of modern silicon integrated microcircuits and other semiconductor devices which have layered structure. For example, it can be helpful for verification of the numerical solutions obtained and for investigation of the features of transport processes of vacancies and silicon self-interstitial atoms depending upon the implantation parameters and parameters of boundary conditions. It follows from a large uncertainty of diffusivity and other transport properties of point defects known from the literature that the analytical solution obtained can successfully replace the numerical solution in modeling a number of technological processes used in the modern microelectronics.

To illustrate the usefulness of the obtained solution, the investigation of the changes in the form and concentration values of distribution of point defects has been carried out for different boundary conditions and two values of the average migration length of diffusing species. The cases of pure thermal generation of point defects within the limits of the layer and generation of nonequilibrium defects due to hydrogen ion implantation have been investigated. It has been shown that there is a strong influence of the surface on the concentration values and the form of distribution of nonequilibrium point defects when the implantation energy decreases.

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